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Analyzing electron-electron correlations at nanoscale: DFT+DMFT

code for nanosystems¹ VOLODYMYR TURKOWSKI, ALAMGIR KABIR, TALAT S. RAHMAN, Physics Department and NSTC, University of Central Florida — We propose a DFT+DMFT approach to study electron-electron correlation effects in nanosized systems containing atoms with localized d- and f-electron states. For the purpose we have developed a nanoDFT+DMFT code which allows one to study the properties of systems containing up to several hundred atoms. The system geometry is first optimized using ab-initio electron structure calculations based on density-functional theory (DFT), and correlation effects are analyzed employing nonhomogeneous Dynamical Mean-Field Theory (DMFT) calculations with the iterated perturbation theory (IPT) approximation for the quantum impurity solver. To test the formalism we have evaluated the magnetic properties of several transition metal atom clusters and compared the results with those obtained from the exact diagonalization method (a few-atom clusters) and available experimental data (2-19 atom clusters). In particular, we find that the IPT-DMFT gives magnetic moments much closer to experimental values as compared to DFT calculations. We discuss possible extensions of the approach including application of more accurate quantum impurity solvers, such as Hirsch-Fye and Continuous-Time Quantum Monte Carlo. The application of the methodology to the nonequilibrium case is in progress.

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